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Spatially-dispersive surface modes on interfaces of layered hyperbolic metamaterials

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Abstract. In this work we present the study of influence of spatial dispersion on the existence of surface modes on the interfaces with multilayered hyperbolic metamaterials (HMMs). To that end we employ operator effective medium approximation correcting the Maxwell Garnett approximation. We find out the strong effect of the layer order on the dispersion of surface waves and reveal the dispersion curves missing in the Maxwell Garnett approximation. It is also shown that due to spatial dispersion layered HMMs can sustain TE-polarized surfaces modes.

INTRODUCTION

Surface modes (waves) are the monochromatic solutions of Maxwell's equations localized at interfaces. Localization stems from the coupling of the electromagnetic wave with the electric charge oscillations at the interface, the coupled states being called surface plasmon polaritons (SPPs) [1]. These propagating surface modes can be applied for biological and chemical sensing. Flat interface between two half-spaces filled with isotropic dielectric and metal is the simplest system that sustains surface modes (SPPs). In this case the SPPs are described by the TM-polarized evanescent electromagnetic waves on both sides of the interface. Propagation constant (tangential wave vector k_t) of a SPP is related to its circular frequency ω via dispersion relation, which is provided by the equality of wave impedances on two sides of the interface and reads

$$k_t = k_0 \sqrt{\frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}}, \tag{1}$$

where $k_0 = \omega/c$ is the vacuum wave number, ε_d (ε_m) is the permittivity of the dielectric (metal).

In this paper we study the surface modes on the interfaces of hyperbolic metamaterials (HMMs). The name of a hyperbolic metamaterial originates from the isofrequency surface shape which is either single- or double-sheeted rotation hyperboloid. Particular interest of scientific community to HMMs is caused by their numerous potential applications. For instance, hyperbolic metamaterials have already been exploited for engineering of Purcell factor to control spontaneous emission rate and overcoming diffraction limit. There are two common realization of HMMs: (1) set of alternating metallic and dielectric slabs of subwavelength thicknesses; (2) array of subwavelength metallic wires embedded into the dielectric matrix. The ease of fabrication of these structures is another reason of popularity of HMMs [2]. We deal with the first realization of a HMM and study surface modes localized on the interface between two half spaces filled with isotropic dielectric of permittivity ε on the one side and a set of alternating layers of isotropic metal and dielectric with permittivities ε_m and ε_d, respectively. Metallic slab has thickness d_m and dielectric slab is of the thickness d_d. Fig. 1 depicts the system.

EFFECTIVE MEDIUM APPROXIMATION

Despite the fact that there is the exact solution of Maxwell's equations for layered periodic structures in the form of Bloch waves, its closed-form analysis is baffling [3]. However, as layers which compose HMMs are much thinner

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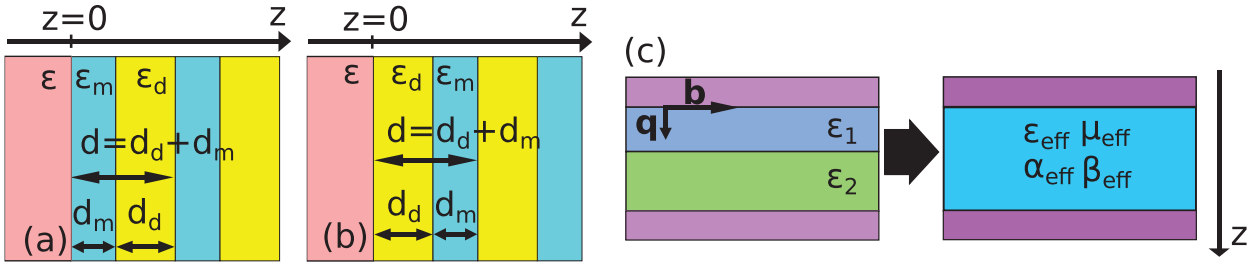

FIGURE 1. Sketch of the system under consideration: the space is filled with isotropic dielectric ($z < 0$) and layered hyperbolic metamaterial ($z > 0$). (a) Regular order, i.e. metallic layer is adjacent to semi-infinite dielectric. (b) Reverse order, i.e. dielectric layer is adjacent to semi-infinite dielectric. (c) Schematic of homogenization procedure of a bi-layered periodic structure characterized by the permittivities ε_1 and ε_2.

than the vacuum wavelength, the description of the multilayer by means of effective medium is possible [3]. Effective medium is based on an apparent fact: albeit the microscopic (atomic) nature of a material is discrete, its interaction with electromagnetic wave can be described in terms of macroscopic parameters such as permittivity and permeability. Thus, it is logical to assume that when characteristic size of the structural inhomogeneity (meta-atom) is small in comparison with the scale of field variation we can assign the effective homogeneous parameters to inhomogeneous structure [4].

To homogenize the layered structure we use the operator effective medium theory (OEMA) developed in [5]. Effective medium of a layered structure schematically depicted in Fig. 1(c) is characterized by permittivity ($\hat{\varepsilon}_{eff}$) and permeability ($\hat{\mu}_{eff}$) tensors and gyration pseudotensors ($\hat{\alpha}_{eff}$ and $\hat{\beta}_{eff}$). In the considered case the material tensors have the following structure

$$\hat{\varepsilon}_{eff} = \varepsilon_o \hat{I} + \varepsilon_e \mathbf{q}\otimes\mathbf{q}, \quad \hat{\mu}_{eff} = \mu_o \hat{I} + \mu_e \mathbf{q}\otimes\mathbf{q}, \quad \hat{\alpha}_{eff} = i\alpha_{TE}\frac{\mathbf{a}\otimes\mathbf{b}}{b^2} + i\alpha_{TM}\frac{\mathbf{b}\otimes\mathbf{a}}{b^2}, \quad \hat{\beta}_{eff} = -\hat{\alpha}_{eff}^T.$$

Here the operator $\hat{I}$ is the projector operator onto the plane of the layers, $\mathbf{q}$ is a unit vector orthogonal to the plane of layers, $\mathbf{b}$ is the tangential wave vector divided by vacuum wavenumber, i.e. $\mathbf{k}_t/k_0$, and $\mathbf{a} = \mathbf{b}\times\mathbf{q}$. Procedure developed in [5] provides expressions for principal components of effective material tensors in the form of the expansion over the small parameter $(k_0 d)$, where $d = d_1 + d_2$. In this study we use OEMA of the second order, i.e. keep the terms up to $(k_0 d)^2$ as follows

$$\varepsilon_o = \varepsilon_o^{(0)} + \frac{(k_0 d)^2}{6}\sigma f(b)\tilde{\varepsilon}_o, \quad \frac{1}{\varepsilon_e} = \frac{1}{\varepsilon_e^{(0)}} + \frac{(k_0 d)^2}{6}\sigma\left(\frac{2\rho-1}{\varepsilon_r} - \frac{f(b)}{\tilde{\varepsilon}_e}\right), \quad \mu_o = 1 + \frac{(k_0 d)^2}{6}\sigma(2\rho-1),$$
$$\frac{1}{\mu_e} = 1 + \frac{(k_0 d)^2}{6}\sigma\left(\rho\frac{\varepsilon_1}{\varepsilon_2} - (1-\rho)\frac{\varepsilon_2}{\varepsilon_1}\right), \quad \alpha_{TE} = \frac{k_0 d}{2}\sigma, \qquad \alpha_{TM} = \frac{k_0 d}{2}\sigma f(b), \tag{2}$$

where

$$f(b) = \frac{b^2}{\varepsilon_r} - 1, \quad \sigma = \rho(1-\rho)(\varepsilon_2 - \varepsilon_1), \quad \tilde{\varepsilon}_o = \rho\varepsilon_1 - (1-\rho)\varepsilon_2, \quad \tilde{\varepsilon}_e = \left(\frac{\rho}{\varepsilon_1} - \frac{1-\rho}{\varepsilon_2}\right)^{-1}.$$

Here $\rho = d_1/d$ is the fill fraction of material 1, $\varepsilon_r = (\varepsilon_1^{-1} + \varepsilon_2^{-1})^{-1}$ is the reduced permittivity, and $\varepsilon_{o,e}^{(0)}$ are effective permittivities of the layered structure in the Maxwell Garnett approximation, i.e.

$$\varepsilon_o^{(0)} = \rho\varepsilon_1 + (1-\rho)\varepsilon_2, \quad \varepsilon_e^{(0)} = \frac{\varepsilon_1\varepsilon_2}{\rho\varepsilon_2 + (1-\rho)\varepsilon_1}. \tag{3}$$

Maxwell Garnett approximation follows from equation (2), when the terms proportional to $(k_0 d)^1$ and $(k_0 d)^2$ are dropped. Being inaccurate in some cases (see for instance [6]), the Maxwell Garnett approximation is widely adopted among researchers due to its simplicity and clearness. The properties of the structure in the first order of OEMA (terms up to $(k_0 d)^1$ are kept) depend on order of layers, i.e. when the stack starts from layer 2 ($1 \leftrightarrow 2$), $\hat{\alpha}_{eff}$ and $\hat{\beta}_{eff}$ change their signs. Therefore we consider two configurations: (i) metallic layer goes first ($\varepsilon_1 = \varepsilon_m$ and $d_1 = d_m$) and (ii) dielectric layer goes first ($\varepsilon_1 = \varepsilon_d$ and $d_1 = d_d$). These two cases are depicted in Figs. 1(a) and (b), respectively. Further we assume dispersionless dielectrics and Drude-model metal as $\varepsilon_m = 1 - (\omega_p/\omega)^2$, where ω_p is the plasma frequency.

DISPERSION RELATIONS FOR SURFACE MODES

It is well known that the system sustains surfaces modes when wave impedances of the waves on different sides of the interface equal. Thus, to obtain dispersion relations for surface modes we equal wave impedances of eigenmodes of effective medium and dielectric below it. To check validity of the effective medium approximation we also solve numerically dispersion equation obtained for initial layered structure.

Eigenwaves of the effective medium are TE- or TM-polarized plane waves while for the initial layered structure they are TE- or TM-polarized Bloch waves. One can easily find the following dispersion relation for effective medium eigenwaves

$$\eta_{TM} = \sqrt{-\alpha_{TM}^2 + \varepsilon_o\mu_o - \varepsilon_o/\varepsilon_e b^2}, \quad \eta_{TE} = \sqrt{-\alpha_{TE}^2 + \varepsilon_o\mu_o - \mu_o/\mu_e b^2}, \tag{4}$$

where η is the longitudinal wavenumber divided over vacuum wavenumber, i.e. k_z/k_0. Wave impedances of eigenwaves of effective medium and isotropic dielectric equal

$$Z_{eff}^{TE} = \frac{\mu_o}{i\alpha_{TE} + \eta_{TE}}, \quad Z_{eff}^{TM} = \frac{i\alpha_{TM} + \eta_{TM}}{\varepsilon_o}, \quad Z_{\varepsilon}^{TE} = \frac{1}{\sqrt{\varepsilon - b^2}}, \quad Z_{\varepsilon}^{TM} = \frac{\sqrt{\varepsilon - b^2}}{\varepsilon}.$$

Wave impedances of Bloch wave in the considered layered structure can be found in [3]. Thus, one arrives at the following dispersion equations for surfaces modes at the interface between isotropic dielectric and effective medium for respectively TE and TM polarization

$$-1 - \frac{\mu_o\sqrt{b^2 - \varepsilon}}{\sqrt{\alpha_{TE}^2 - \varepsilon_o\mu_o + \mu_o/\mu_e b^2}} = \frac{\alpha_{TE}}{\sqrt{\alpha_{TE}^2 - \varepsilon_o\mu_o + \mu_o/\mu_e b^2}}, \tag{5}$$

$$\varepsilon_o + \frac{\varepsilon}{\sqrt{b^2 - \varepsilon}}\alpha_{TM} = -\frac{\varepsilon}{\sqrt{b^2 - \varepsilon}}\sqrt{\frac{\varepsilon_o}{\varepsilon_e}}\sqrt{\alpha_{TM}^2\frac{\varepsilon_e}{\varepsilon_o} - \varepsilon_e\mu_o + b^2}. \tag{6}$$

It is interesting to compare surface modes dispersion within the second order of OEMA and Maxwell Garnett approximation. For the case of TM polarization dispersion equation (6) in Maxwell Garnett approximation reduces to

$$b^2 = \varepsilon\frac{\varepsilon_e^{(0)}(\varepsilon_o^{(0)} - \varepsilon)}{\varepsilon_e^{(0)}\varepsilon_o^{(0)} - \varepsilon^2}. \tag{7}$$

In the same time the Maxwell Garnett approximation does not predict the existence of TE-polarized surface modes while equation (5) can have solutions due to the magnetoelectric coupling facilitating excitation of surface modes. However, it is important to understand that these TE polarized surface modes are not associated with induced surface charge in strong contrast to TM polarized modes. From equation (7) one arrives at the conclusion that the surface mode exists when either $\varepsilon_e^{(0)}\varepsilon_o^{(0)} < 0$ and $b^2 < \varepsilon_e^{(0)}$ or $\varepsilon_o^{(0)} < 0$ and $\varepsilon_e^{(0)} < 0$. In the first case the structure exhibits hyperbolic behavior and excited surface modes are called *virtual SPPs*. In the second case the structure is just an anisotropic metal, while the surface modes are the *usual SPPs*. This terminology is borrowed from [7].

As Fig. 2 clearly demonstrates, the dispersion of surface modes strongly depends on the order of layers and metal fill fraction. It also shows that the 2nd order of OEMA is in perfect agreement with the exact solution for initial layered structures and can be used to interpret behavior of surface modes dispersion. Striking differences between SPPs in the case of uniaxial crystal (here represented by HMM in Maxwell Garnett approximation, see Figs. 2(a) and (b)) and layered structure are caused by the spatial dispersion usual SPPs can exist even though the structure exhibits a "dielectric" behavior, i.e. when $\varepsilon_o > 0$ and $\varepsilon_e > 0$, while for virtual SPPs a completely new branch of the dispersion curve exists. It is characterized by large tangential wave vectors [cf. Figs. 2(a) and (c)]. Spatial dispersion can also lead to truncation of dispersion curve as it is observed from Fig. 2(f), while metallic uniaxial crystal would sustain SPPs (see Fig. 2(b)). We think about surface modes existing when the HMM exhibits "dielectric" behavior as they are were SPPs because in terms of OEMA polarization of the medium is caused by both electric and magnetic fields and it is not completely correct to make conclusions about its "dielectric" behavior based only on permittivity. Moreover, due to discontinuity of normal component of electric field there is surface charge coupled to electromagnetic wave.

In qualitative way the strongest influence on surface modes dispersion has parameter of gyrotropy α_{TM} which changes its sign when either order of layers is changed or tangential wave number of surface mode exceeds that of SPP described by (1).

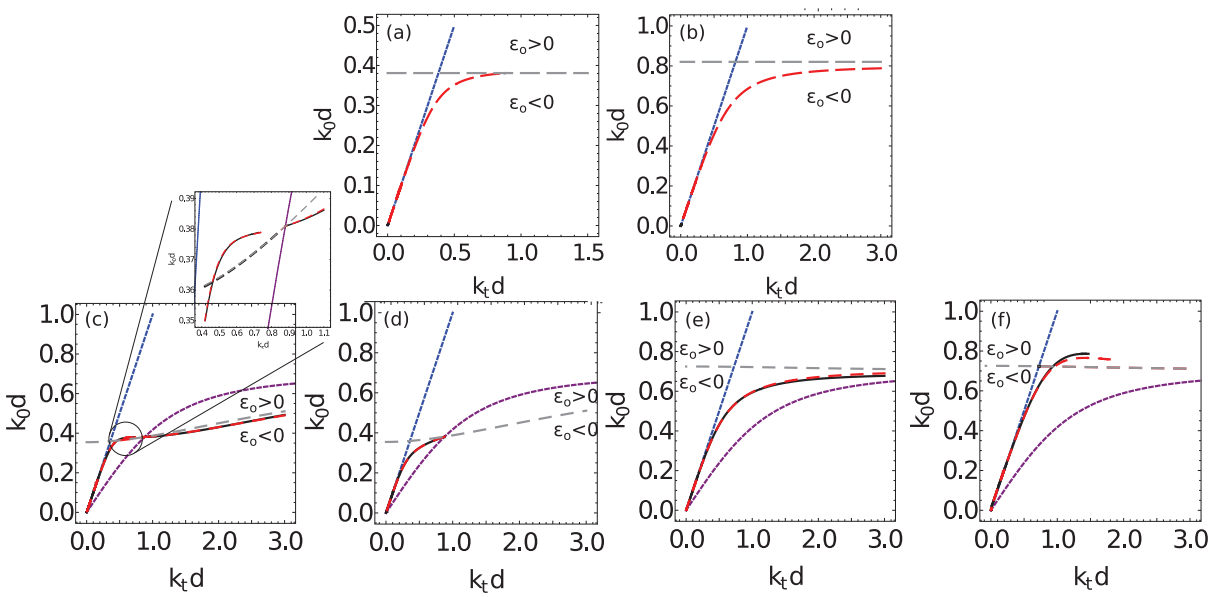

FIGURE 2. Dispersion curves of TM surface modes on the interface with the effective media (red dashed curves) and layered structures (black curves). Blue dashed line is the light line. Gray are defined by $\varepsilon_o = 0$. Purple curve corresponds to the dispersion curve given by Eq. (1) of SPP at the interface between half spaces with ε_d and ε_m. (a) Virtual SPP ($\rho = 0.2$) and (b) usual SPP ($\rho = 0.6$) in Maxwell Garnett approximation. (c) Regular order ($\sigma > 0$), $\rho = 0.2$, (d) reverse order ($\sigma < 0$), $\rho = 0.2$, (e) reverse order ($\sigma < 0$), $\rho = 0.6$ and (f) regular order ($\sigma > 0$), $\rho = 0.6$ for the HMM within the second order OEMA. Plasma frequency $\omega_p = \pi c/(2d)$ corresponds to vacuum wavelength $\lambda_p = 4d$, permittivity of dielectric slab is $\varepsilon_d = 4$, and permittivity of dielectric half space is $\varepsilon = 1$.

In conclusion, we have applied effective medium theory developed within OEMA to study dispersion peculiarities of surface modes at the interface between dielectric half space and semi-infinite layered HMMs. It is possible to classify surface modes in terms of virtual and usual SPPs as it is done for uniaxial crystals in [7], for instance. We reveal the strongest dependence of surface modes dispersion on the order of layers and existence of dispersion curve branches absent in Maxwell Garnett approximation. We also provide dispersion equation for TE-polarized surface modes which has nontrivial solutions.

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